

# Stochasticity, decoherence and an arrow of time from the discretization of time?

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Certain intriguing consequences of the discreteness of time on the time evolution of dynamical systems are discussed. In the discrete-time classical mechanics proposed here, there is an *arrow of time* that follows from the fact that the replacement of the time derivative by the backward difference operator alone can preserve the non-negativity of the phase space density. It is seen that, even for free particles, all the degrees of freedom are *correlated* in principle. The forward evolution of functions of phase space variables by a finite number of time steps, in this discrete-time mechanics, depends on the entire continuous-time history in the interval  $[0, \infty]$ . In this sense, discrete time evolution is *nonlocal* in time from a continuous-time point of view. A corresponding quantum mechanical treatment is possible *via* the density matrix approach. The interference between non-degenerate quantum mechanical states decays exponentially. This *decoherence* is present, in principle, for all systems; however, it is of practical importance only in macroscopic systems, or in processes involving large energy changes.

## INTRODUCTION

*Time* is an enigma, and many philosophers and scientists have tried to ponder over its true meaning. However, most physicists and mathematicians consider the concepts of space and time to be intuitively obvious, and view space-time as an inert and infinitely divisible continuum in which ‘events’ unfold. The advent of the general theory of relativity led to the insight that space-time is dynamical and that the gravitational field should be identified with certain properties of the space-time continuum. Subsequent efforts at synthesizing gravity and quantum mechanics, either with a background space as in string theory [1], or without a background space as in loop quantum gravity [2, 3], strongly suggest that space-time at the most fundamental level has a granular nature. In loop quantum gravity, the spatial Riemannian geometry is discrete [4] with the volume of space quantized in units of  $l_p^3$ , where the Planck length  $l_p = (\hbar G/c^3)^{1/2} \approx 1.6 \times 10^{-35}$  m. Further, the time evolution takes place in discrete time steps [5] of the order of the Planck time  $t_p = (\hbar G/c^5)^{1/2} \approx 5.4 \times 10^{-44}$  s.

There have been some attempts in the literature [6, 7, 8, 9, 10] to study the time evolution of Hamiltonian systems with time as a discrete parameter even before these exciting developments took place. In particular, Katayama and Yukawa argued that, just like matter, space-time also should have an indivisible element (an ‘elementary domain’). Yamamoto [10] also made an attempt to realize the elementary domain through quantum field theory in discrete time. In this paper, we propose a version of discrete-time mechanics as a precursor to the more complicated (and conceptually satisfying) discrete space-time mechanics. The idea is to explore the genuine consequences of discrete-time evolution, and not the development of numerical methods to approximate continuous-time evolution with greater precision. In the equation of motion approach to classical mechanics (CM), Lee [11, 12] found that violation of time-translational invariance (that accompanies discretization of time) leads to non-conservation of energy. He therefore developed a theory with time as a discrete dynamical variable. Subsequently, Jaroszkiewicz and coworkers [13] succeeded in developing an equation of motion approach to CM with time as a discrete parameter by invoking the discrete-time action principle of Cadzow [14].

We take a fresh look at the problem and adopt the phase space density approach. We start with the Liouville equation for the phase space density in classical mechanics, and propose its discrete-time analogue. The structure of this discrete-time Liouville equation ensures that *all* the constants of the motion in continuous-time mechanics are also constants of the motion in discrete-time mechanics. The basic premises that underlie the derivation of this equation and the consequences of the discreteness of time (the emergence of stochasticity, correlation and non-locality) are discussed in Section 2. The mathematical details are relegated to Appendices A and B. We then quantize the discrete-time Liouville equation to obtain the time evolution of the Wigner distribution function (equivalently, the density matrix). It is seen that the discretization of time leads to energy super-selection and decoherence. These points are discussed in Section 3. Even though the present formalism is motivated by Hamiltonian mechanics, we have attempted to study the consequences of discrete time on more general forms of dynamical systems. In particular, the effect of the discreteness of time on the sensitive dependence on initial conditions of (chaotic) nonlinear dynamical

systems is discussed briefly in Section 4. Finally, some conclusions are drawn in Section 5. Before we proceed, we would like to emphasize that the fundamental unit of time  $\tau$  that appears in our formalism need *not* be equal to the Planck time. We also remark that the usual continuous-time mechanics is recovered in the limit  $\tau \rightarrow 0$ .

### CLASSICAL MECHANICS IN DISCRETE TIME

We consider a dynamical system with  $l$  degrees of freedom described by the Hamiltonian  $H(\vec{x}, \vec{p})$ , where  $x_i$  and  $p_i$  are the coordinates and canonical momenta, respectively. The time evolution of the phase space density  $\rho_{\text{ct}}(\vec{x}, \vec{p}, t)$  is given by the Liouville equation

$$\frac{\partial}{\partial t} \rho_{\text{ct}}(\vec{x}, \vec{p}, t) = \{H, \rho_{\text{ct}}\} = L \rho_{\text{ct}}(\vec{x}, \vec{p}, t) \quad (1)$$

where  $\{H, \rho_{\text{ct}}\}$  is the Poisson bracket of  $H$  with  $\rho_{\text{ct}}(\vec{x}, \vec{p}, t)$ , and  $L$  is the Liouville operator

$$L = \sum_{i=1}^l \left( \frac{\partial H}{\partial x_i} \frac{\partial}{\partial p_i} - \frac{\partial H}{\partial p_i} \frac{\partial}{\partial x_i} \right).$$

Throughout this paper, the suffixes ‘ct’ and ‘dt’ as in  $F_{\text{ct}}$  and  $F_{\text{dt}}$  shall denote values of the phase space function  $F$  in continuous-time mechanics and discrete-time mechanics, respectively. The formal solution of Eq. (1) is given by

$$\rho_{\text{ct}}(\vec{x}, \vec{p}, t) = e^{tL} \rho_{\text{ct}}(\vec{x}, \vec{p}, 0) \quad (2)$$

where  $\rho_{\text{ct}}(\vec{x}, \vec{p}, 0)$  is the initial phase space density. Throughout this paper, we consider the deterministic initial condition

$$\rho_{\text{ct}}(\vec{x}, \vec{p}, 0) = \delta(\vec{x} - \vec{x}(0)) \delta(\vec{p} - \vec{p}(0)). \quad (3)$$

The value  $F_{\text{ct}}(t)$  of the phase space function  $f(\vec{x}, \vec{p})$  at time  $t$  is given by

$$F_{\text{ct}}(t) = \langle f(\vec{x}, \vec{p}) \rangle_{\text{ct}} = \int d\vec{x} \int d\vec{p} f(\vec{x}, \vec{p}) \rho_{\text{ct}}(\vec{x}, \vec{p}, t).$$

Our aim is to “deduce” the discrete-time analogue of Eq. (1). Since there is no unique definition of a discrete time derivative, we do this by first stipulating the conditions to be satisfied by the equation that governs the time evolution of the phase space density  $\rho_{\text{dt}}(\vec{x}, \vec{p}, n)$  at discrete time  $t = n\tau$ , where  $\tau$  is the fundamental unit of time. Specifying the data at one instant of time is sufficient to obtain the solution of Eq. (1). We demand that specifying  $\rho_{\text{dt}}(\vec{x}, \vec{p}, j)$  at some discrete time  $t = j\tau$  should be sufficient to determine  $\rho_{\text{dt}}(\vec{x}, \vec{p}, j')$  at any other discrete time  $t' = j'\tau$ . This implies that the equation to be discovered should essentially be a first-order difference equation in time. We thus obtain the most general form of the discrete-time Liouville equation for forward evolution in the form

$$\frac{\rho_{\text{dt}}(\vec{x}, \vec{p}, n+1) - \rho_{\text{dt}}(\vec{x}, \vec{p}, n)}{\tau} = L [\alpha \rho_{\text{dt}}(\vec{x}, \vec{p}, n) + \beta \rho_{\text{dt}}(\vec{x}, \vec{p}, n+1)], \quad (4)$$

where  $0 \leq \alpha, \beta \leq 1$  and  $\alpha + \beta = 1$ . Special cases of Eq. (4) are the forward and backward difference schemes obtained from Eq. (4) by setting  $\alpha = 1$  and  $\alpha = 0$ , respectively. Restrictions on the possible values of  $\alpha$  can be obtained by examining the time evolution operator  $T_n$  defined through the equation

$$\rho_{\text{dt}}(\vec{x}, \vec{p}, n) = \left( \frac{1 + \alpha\tau L}{1 - \beta\tau L} \right)^n \rho_{\text{dt}}(\vec{x}, \vec{p}, 0) = T_n \rho_{\text{dt}}(\vec{x}, \vec{p}, 0). \quad (5)$$

We assume that the Hamiltonian and the manifold in which the dynamics takes place are such that  $L$  is sufficiently well defined.  $L$  is then a skew-Hermitian operator, and hence its spectrum is pure imaginary. Using the relation

$$\int f(\vec{\Omega}) [G(L)g(\vec{\Omega})] d\vec{\Omega} = \int [G(-L)f(\vec{\Omega})] g(\vec{\Omega}) d\vec{\Omega}$$

where  $\vec{\Omega} = (\vec{x}, \vec{p})$ , we can show that every quantity that is conserved in the continuous time context is also conserved under the time evolution scheme proposed here.

It is clear that it is only when  $\alpha = \frac{1}{2}$  that  $T_n$  is unitary and the evolution given by Eq. (5) is consistent with time reversal invariance.  $T_n$  is an unbounded operator (a bounded function would evolve to an unbounded one under the action of  $T_n$ ) in the limit  $n \rightarrow \infty$  for  $\alpha > \frac{1}{2}$ . Since this is undesirable,  $\alpha$  must be less than  $\frac{1}{2}$  for  $n > 0$ . Similarly,  $T_n$  is unbounded in the limit  $n \rightarrow -\infty$  for  $\alpha < \frac{1}{2}$ . Hence  $\alpha$  must be greater than  $\frac{1}{2}$  for  $n < 0$ . Thus, an arrow of time emerges naturally if  $\alpha \neq \frac{1}{2}$ .

A more stringent constraint on the value of  $\alpha$  can be obtained by demanding that the phase space density  $\rho_{\text{dt}}(\vec{x}, \vec{p}, n)$  be *non-negative*. We examine this problem in two different ways, and show that zero is the only permissible value of  $\alpha$ .

### Method 1:

Let us make a formal transformation

$$(x_1, \dots, x_l; p_1, \dots, p_l) \rightarrow (\xi_1, \dots, \xi_l; \eta_1, \dots, \eta_l),$$

such that  $L = -\partial/\partial\xi_1$ . This transformation can be worked out explicitly for systems with quadratic Hamiltonians. While global realization of such a transformation for systems with non-quadratic Hamiltonians appears to be doubtful, the analysis is instructive, and we proceed with it. For the deterministic initial condition Eq. (3), the corresponding initial condition in the transformed variables is given by

$$\bar{\rho}_{\text{dt}}(\vec{\xi}, \vec{\eta}, 0) = \prod_{i=1}^l \delta(\xi_i - \xi_i(0)) \delta(\eta_i - \eta_i(0)).$$

The time evolution of  $\bar{\rho}_{\text{dt}}(\vec{\xi}, \vec{\eta}, n)$  is given by Eq. (5) to be

$$\bar{\rho}_{\text{dt}}(\vec{\xi}, \vec{\eta}, n) = g_n(\xi_1) \delta(\eta_1 - \eta_1(0)) \prod_{i=2}^l \delta(\xi_i - \xi_i(0)) \delta(\eta_i - \eta_i(0)),$$

where

$$g_n(\xi_1) = \left( \frac{1 - \alpha\tau \partial/\partial\xi_1}{1 + \beta\tau \partial/\partial\xi_1} \right)^n \delta(\xi_1 - \xi_1(0)).$$

As shown in Appendix A, we find that zero is the only allowed value of  $\alpha$  which renders  $\bar{\rho}_{\text{dt}}(\vec{\xi}, \vec{\eta}, n)$  non-negative and  $T_n$  bounded. For this case, a simple expression can be derived for  $g_n(\xi_1)$ , namely,

$$g_n(\xi_1) = \begin{cases} \frac{1}{(n-1)!\tau} \left( \frac{\xi_1 - \xi_1(0)}{\tau} \right)^{n-1} \exp\left(-\frac{\xi_1 - \xi_1(0)}{\tau}\right), & \text{for } \xi_1 > \xi_1(0) \\ 0, & \text{for } \xi_1 < \xi_1(0). \end{cases} \quad (6)$$

We thus see that the backward difference scheme is the only acceptable generalization of the time derivative to the discrete domain.

### Method 2:

Here we obtain a relation between  $\rho_{\text{ct}}(\vec{x}, \vec{p}, t)$  and  $\rho_{\text{dt}}(\vec{x}, \vec{p}, n)$  by resorting to the generating function technique. As shown in Appendix B, we arrive at the same conclusion: namely, that zero is the only permissible value of  $\alpha$  that renders  $\rho_{\text{dt}}(\vec{x}, \vec{p}, n)$  non-negative. This analysis leads to the following intriguing relation for  $n > 0$ :

$$\rho_{\text{dt}}(\vec{x}, \vec{p}, n) = \frac{1}{(n-1)!} \int_0^\infty du e^{-u} u^{n-1} \rho_{\text{ct}}(\vec{x}, \vec{p}, \tau u). \quad (7)$$

The average value  $F_{\text{dt}}(n)$  of any function  $f(\vec{x}, \vec{p})$  at time  $t = n\tau$  is given by

$$F_{\text{dt}}(n) = \langle f(\vec{x}, \vec{p}) \rangle_{\text{dt}, n} = \frac{1}{(n-1)!} \int_0^\infty du e^{-u} u^{n-1} F_{\text{ct}}(\tau u), \quad (8)$$

where  $F_{ct}(\tau u)$  is the phase space average in continuous-time mechanics at time  $t = \tau u$ . Such quantities are *nonlocal* in time from the continuous-time point of view! The discreteness of space-time thus leads to non-locality in time in this sense.

Both Eqs. (6) and (7) imply that an element of stochasticity appears in the discrete-time classical mechanics described in this paper. Equation (6) suggests that the stochasticity is essentially in one variable,  $\xi_1$ , and that its conditional probability density is a gamma distribution for all Hamiltonian systems. Equation (7) implies a random walk in time. Thus  $\xi_1$  can be identified with a kind of “internal time”.

### Examples

We now illustrate the peculiarities of discrete-time evolution with the help of two examples: (i) a collection of free particles, and (ii) a collection of harmonic oscillators.

#### (i) Free particles:

For a collection of free particles described by the Hamiltonian  $H = \sum_{i=1}^l p_i^2/(2m_i)$  with deterministic initial conditions, we get the following results for the averages of  $x_i$ ,  $p_i$ ,  $x_i^2$  and  $p_i^2$  at discrete time  $n\tau$ :

$$\langle x_i \rangle_{\text{dt},n} = x_i(0) + \frac{p_i(0)n\tau}{m_i}, \quad \langle p_i \rangle_{\text{dt},n} = p_i(0),$$

$$\langle x_i^2 \rangle_{\text{dt},n} = \left( x_i(0) + \frac{p_i(0)n\tau}{m_i} \right)^2 + \frac{np_i^2(0)\tau^2}{m_i^2}, \quad \langle p_i^2 \rangle_{\text{dt},n} = p_i^2(0).$$

Since  $\langle p_i^2 \rangle_{\text{dt},n} = p_i^2(0)$ ,  $H$  is conserved. However,

$$\langle x_i^2 \rangle_{\text{dt},n} - \langle x_i \rangle_{\text{dt},n}^2 = n \frac{p_i^2(0)\tau^2}{m_i^2} = D_i t$$

where  $D_i = p_i^2(0)\tau/m_i^2$ . Hence the motion of the particles is *diffusive*. A similar calculation shows that

$$\langle x_i x_j \rangle_{\text{dt},n} - \langle x_i \rangle_{\text{dt},n} \langle x_j \rangle_{\text{dt},n} = n \frac{p_i(0)p_j(0)\tau^2}{m_i m_j},$$

which implies that even the motion of *non-interacting* particles is correlated in the foregoing sense.

#### (ii) Harmonic oscillators:

Next, consider a collection of harmonic oscillators described by the Hamiltonian  $H = \sum_{i=1}^l \frac{1}{2}(p_i^2 + x_i^2)$ , where we have taken all the masses and frequencies to be identical and set  $m_i = 1$ ,  $\omega_i = 1$ , for simplicity. The analysis of this case is straightforward. The final expressions for the first and second moments of  $x_i$  and  $p_i$  at time  $n\tau$  are

$$\langle x_i \rangle_{\text{dt},n} = \frac{r_i(0)}{(1 + \tau^2)^{n/2}} \sin(n\phi + \theta_i(0)),$$

$$\langle p_i \rangle_{\text{dt},n} = \frac{r_i(0)}{(1 + \tau^2)^{n/2}} \cos(n\phi + \theta_i(0)),$$

$$\langle x_i^2 \rangle_{\text{dt},n} = \frac{r_i^2(0)}{2} \left[ 1 + \frac{\cos(n\phi' + 2\theta_i(0))}{(1 + 4\tau^2)^{n/2}} \right],$$

$$\langle p_i^2 \rangle_{\text{dt},n} = \frac{r_i^2(0)}{2} \left[ 1 - \frac{\cos(n\phi' + 2\theta_i(0))}{(1 + 4\tau^2)^{n/2}} \right],$$

$$\langle x_i x_j \rangle_{\text{dt},n} = \frac{r_i(0)r_j(0)}{2} \left[ \cos(\theta_i(0) - \theta_j(0)) + \frac{\cos(n\phi' + \theta_i(0) + \theta_j(0))}{(1 + 4\tau^2)^{n/2}} \right],$$

where  $\phi = \arctan \tau$ ,  $\phi' = \arctan(2\tau)$ ,  $r_i^2 = x_i^2 + p_i^2$ , and  $\theta_i = \arctan(x_i/p_i)$ . We see that  $\langle x_i^2 \rangle_{\text{dt},n} - \langle x_i \rangle_{\text{dt},n}^2$  and  $\langle p_i^2 \rangle_{\text{dt},n} - \langle p_i \rangle_{\text{dt},n}^2$  are nonzero, signalling stochasticity in  $x_i$  and  $p_i$ . However, the Hamiltonian  $H$  is conserved. We also see that  $\langle x_i x_j \rangle_{\text{dt},n} - \langle x_i \rangle_{\text{dt},n} \langle x_j \rangle_{\text{dt},n}$  is nonzero, implying that all the degrees of freedom are now correlated.

## QUANTUM MECHANICS IN DISCRETE TIME

Quantum mechanics (QM) is a remarkably successful theory with no known physical phenomena that contradict it. Yet, it has no universally accepted interpretation and hence the adage, “It is a theory that works for all practical purposes” [15]. The founding fathers of QM have insisted that the results of *measurements* have to be expressed in classical terms. If the world is quantum mechanical, then classical mechanics (CM) should be contained within QM as a limiting case. Now, a crucial ingredient of QM is the principle of superposition that follows from the linearity of the Hilbert space. Even though manifestations of quantum mechanical interference abound in the microscopic domain, the application of such a principle to the macro-world seems to lead to predictions that are counter-intuitive *vis-à-vis* our day-to-day experience. The Schrödinger cat paradox, invented by Schrödinger himself, clearly brings these issues into focus, and it suggests that, from among the multitude of superpositions allowed by the Schrödinger equation, only a few robust states are allowed for macroscopic systems. The so-called *decoherence program* [16, 17, 18, 19] shows how this may come about entirely within a quantum mechanical description, by invoking the unavoidable interaction of any given system with the external world. Entanglement between the system and the environment can cause super-selection, *i.e.*, the selection of a preferred set of states that are robust in spite of their immersion into the environment. Another consequence of the entanglement is environment-induced decoherence, which refers to the suppression of interference between the preferred states chosen by the super-selection rule. In what follows, we show how energy super-selection and decoherence may arise from the discretization of time.

In continuous time, the density matrix  $\hat{\rho}_{\text{ct}}(t)$  satisfies the well known evolution equation

$$\frac{\partial}{\partial t} \hat{\rho}_{\text{ct}}(t) = \frac{1}{i\hbar} [\hat{H}, \hat{\rho}_{\text{ct}}(t)],$$

where  $\hat{H}$  is the Hamiltonian operator and  $[\hat{A}, \hat{B}]$  is the commutator of the operators  $\hat{A}$  and  $\hat{B}$ . The usual quantization prescriptions whereby  $\rho_{\text{ct}} \rightarrow \hat{\rho}_{\text{ct}}$  and the Poisson bracket  $\{A, B\} \rightarrow [\hat{A}, \hat{B}]/(i\hbar)$ , together with the procedure for going from continuous to discrete time (described in this paper), leads to the following evolution equation for the discrete-time density matrix  $\hat{\rho}_{\text{dt}}(n)$ :

$$\frac{\hat{\rho}_{\text{dt}}(n+1) - \hat{\rho}_{\text{dt}}(n)}{\tau} = \frac{1}{i\hbar} [\hat{H}, \hat{\rho}_{\text{dt}}(n+1)] = \hat{L} \hat{\rho}_{\text{dt}}(n+1)$$

for  $n > 0$ . This implies that

$$\hat{\rho}_{\text{dt}}(n) = \left(1 - \tau \hat{L}\right)^{-n} \hat{\rho}_{\text{dt}}(0).$$

Let  $|\alpha\rangle$  denote the eigenfunction of  $\hat{H}$  with the eigenvalue  $\epsilon_\alpha$ , and  $\hat{\rho}_{\text{dt}}(0)$  the initial density matrix:

$$\hat{H}|\alpha\rangle = \epsilon_\alpha|\alpha\rangle, \quad \hat{\rho}_{\text{dt}}(0) = \sum_{\alpha,\beta} a_{\alpha,\beta} |\alpha\rangle\langle\beta|.$$

We then get

$$\hat{\rho}_{\text{dt}}(n) = \sum_{\alpha,\beta} a_{\alpha,\beta} \left[ 1 + i\tau \left( \frac{\epsilon_\alpha - \epsilon_\beta}{\hbar} \right) \right]^{-n} |\alpha\rangle\langle\beta|.$$

It is clear that the diagonal elements of  $\hat{\rho}_{\text{dt}}(n)$  are time-invariant. The off-diagonal elements decay exponentially if the basis states are non-degenerate. They are, however, time invariant if the states  $|\alpha\rangle$  and  $|\beta\rangle$  are degenerate.

We thus find that, in principle, the interference involving states with different energies decays exponentially with a characteristic time  $T_d$  given by

$$T_d = (2\tau) / \log [1 + (\Delta E \tau / \hbar)^2],$$

where  $\Delta E$  is the difference in energy between the states. If  $\tau$  is taken to be the Planck time ( $5.4 \times 10^{-44}$  s), we find the decay time to be greater than  $10^{10}$  years if  $\Delta E > 7$  meV. Thus, a microscopic system prepared in a mixed state by superposing states separated in energy by a few meV, decoheres only in principle, and continues to be coherent in practice. However, for a macroscopic system with about  $10^{20}$  particles,  $T_d \sim 10^{-23}$  s for states with a 7 meV change in the energy per particle.

The formalism described in this paper can be extended to quantum mechanical distribution functions (QDF) as well. In view of the non-uniqueness associated with the classical  $\leftrightarrow$  quantum correspondence (i.e., the way to construct quantum mechanical operators corresponding to classical phase space functions), there are many ways of defining QDFs [21]. We restrict ourselves to the Wigner distribution function, which follows from the Weyl correspondence rule. We can obtain a quantum mechanical description in discrete time by Wigner-Moyal quantization of the discrete-time Liouville equation. This is achieved by simply replacing the Poisson bracket by the Moyal bracket. The time evolution of the discrete-time Wigner distribution function  $W_{dt}(\vec{x}, \vec{p}, n)$  is given by the backward difference equation

$$\frac{W_{dt}(\vec{x}, \vec{p}, n+1) - W_{dt}(\vec{x}, \vec{p}, n)}{\tau} = H \left( \frac{2}{\hbar} \sin \left[ \frac{\hbar}{2} \overleftrightarrow{\nabla} \right] \right) W_{dt}(\vec{x}, \vec{p}, n+1),$$

where  $\overleftrightarrow{\nabla}$  is the operator defined through the relation

$$A \overleftrightarrow{\nabla} B = \{A, B\}.$$

It may be noted that Eq. (7) holds good in the context of quantum mechanics as well, with the replacements  $\rho_{ct}(\vec{x}, \vec{p}, t) \rightarrow \hat{\rho}_{ct}(t)$  and  $\rho_{dt}(\vec{x}, \vec{p}, n) \rightarrow \hat{\rho}_{dt}(n)$  for the density matrix, and  $\rho_{ct}(\vec{x}, \vec{p}, t) \rightarrow W_{ct}(\vec{x}, \vec{p}, t)$  and  $\rho_{dt}(\vec{x}, \vec{p}, n) \rightarrow W_{dt}(\vec{x}, \vec{p}, n)$  for the Wigner distribution function.

### Connection with the Schrödinger equation

It is interesting to ask if there exists a discrete-time Schrödinger equation whose solution is consistent with the time evolution of the density matrix described in this paper. If such an equation exists, then the eigenstate  $|\alpha\rangle$  should evolve to  $|\alpha\rangle_n = f(n, \alpha) |\alpha\rangle$ , where  $f(n, \alpha)$  is an unknown function that should satisfy the relation

$$f(n, \alpha) f^*(n, \beta) = \left[ 1 + i\tau \left( \frac{\epsilon_\alpha - \epsilon_\beta}{\hbar} \right) \right]^{-n}. \quad (9)$$

When  $\alpha = \beta$ , Eq. (9) reduces to  $|f(n, \alpha)|^2 = 1$ , which implies that  $f(n, \alpha)$  is unimodular: thus  $f(n, \alpha) = \exp[i\Theta(n, \alpha)]$ , where  $\Theta(n, \alpha)$  is a real number. When this expression for  $f(n, \alpha)$  is substituted in Eq. (9), we get

$$\Theta(n, \alpha) - \Theta(n, \beta) = n \arctan \left( \frac{\tau(\epsilon_\alpha - \epsilon_\beta)}{\hbar} \right) + i \frac{n}{2} \log \left[ 1 + \left( \frac{\tau(\epsilon_\alpha - \epsilon_\beta)}{\hbar} \right)^2 \right],$$

in which the left-hand side is real, whereas the right-hand side is complex unless  $\tau = 0$ . Thus the functional equation (9) does not have a solution, and hence we do not have a discrete-time Schrödinger equation consistent with the equation for the density matrix. This is logically consistent with the fact that the density matrix description predicts decoherence, which never can occur in the Schrödinger formalism for an isolated system.

### NONLINEAR DYNAMICS IN DISCRETE TIME

We have so far concentrated on the classical and quantum mechanics of Hamiltonian systems. However, we do encounter more general dynamical systems while modeling numerous phenomena in physics, chemistry and biology. It would be of interest, therefore, to extend the prescription (for going from continuous time to discrete time evolution)

outlined in this paper to dynamical systems described by the set of (in general, nonlinear) ordinary differential equations

$$\frac{d}{dt}x_j(t) = f_j(\{x_i\}), \quad j = 1, \dots, n.$$

We have the equivalent phase space formulation

$$\frac{\partial}{\partial t}\rho_{\text{ct}}(\{x_i\}, t) = L\rho_{\text{ct}}(\{x_i\}, t) = -\sum_{j=1}^n \frac{\partial}{\partial x_j} [f_j(\{x_i\})\rho_{\text{ct}}(\{x_i\}, t)].$$

We note that, presented in this form, there is no obvious distinction between linear and nonlinear equations of motion (the differences between them would be reflected in the spectral properties of the Liouville operator). As a matter of fact, finite-dimensional nonlinear differential equations of motion can be reformulated as linear differential equations in infinite dimensions by adopting the Carleman embedding procedure[20] or similar ones. However, from a practical point of view, there are significant differences between linear and nonlinear problems. Of particular interest is the tendency of nonlinear systems to show chaotic behaviour — *bounded and aperiodic evolution which shows sensitive dependence on initial conditions*. In view of the formula (see Eq. (8)) that relates forward evolution in discrete time to the entire continuous-time history in the semi-infinite interval  $[0, \infty]$ , it is intuitively clear that sensitive dependence on initial conditions in discrete-time mechanics should be different from that of continuous-time mechanics. Some sort of “rounding off” of the instability should occur in the discrete time context, at least in some systems that show bounded evolution, as the following example would suggest.

Let the continuous-time solution for one of the dynamical variables,  $x$ , with initial value  $a$ , be given by the relation

$$x_{\text{ct}}(a, t) = \cos(b e^{ct}), \quad \text{with } x_{\text{ct}}(a, 0) = \cos b = a, \quad (10)$$

where  $c > 0$ . The motion described by Eq. (10) is bounded for all finite  $t$ ; however, it shows sensitive dependence on initial conditions. The ratio of the distance  $d_{\text{ct}}(t)$  between two trajectories emanating from two infinitesimally close-by points  $(a + \Delta)$  and  $a$  is given by

$$d_{\text{ct}}(t) = \left| \frac{x_{\text{ct}}(a + \Delta, t) - x_{\text{ct}}(a, t)}{\Delta} \right| = \left| \frac{\partial x_{\text{ct}}(a, t)}{\partial a} \right|$$

to the first order in  $\Delta$ . It is easily seen that

$$d_{\text{ct}}(t) = \frac{1}{\sqrt{1-a^2}} |\sin(b e^{ct})| e^{ct},$$

so that the Lyapunov exponent

$$\lim_{t \rightarrow \infty} \frac{1}{t} \log(d_{\text{ct}}(t)) = c$$

is positive, signaling chaos. Using Eq. (8), the corresponding expression for the distance in the discrete-time problem is

$$d_{\text{dt}}(n) = \left| \frac{\partial}{\partial a} x_{\text{dt}}(n) \right| = \frac{1}{\sqrt{1-a^2}} \frac{1}{(n-1)!} \left| \int_0^\infty du u^{n-1} e^{-u} e^{c\tau u} \sin(b e^{c\tau u}) \right|.$$

Integrating once by parts, we get

$$d_{\text{dt}}(n) = \frac{1}{\sqrt{1-a^2}} \frac{1}{b c \tau} \frac{1}{(n-1)!} \left| \int_0^\infty du \cos(b e^{c\tau u}) [(n-1)u^{n-2} - u^{n-1}] e^{-u} \right|.$$

Using the fact that  $\left| \int_0^\infty du \cos(b e^{c\tau u}) f(u) \right| \leq \int_0^\infty du |f(u)|$ , we get

$$d_{\text{dt}}(n) \leq \frac{2}{b c \tau} \frac{1}{\sqrt{1-a^2}},$$

which is bounded for all times. Thus the Lyapunov exponent for the discrete time evolution vanishes for this example.

In order to get a feel for the differences between discrete and continuous time mechanics, let us consider a few more examples. If the equations of motion are such that  $x_{\text{ct}}(t) \sim t^\alpha$  (with  $\alpha > -1$ ), then the corresponding discrete time evolution is given by  $x_{\text{dt}}(n) \sim \tau^\alpha \Gamma(n + \alpha)/(n - 1)!$  which goes as  $(n\tau)^\alpha$  for  $n \gg \alpha$ . That is, a system that shows power law evolution in continuous time shows similar behaviour in discrete-time mechanics. If  $x_{\text{ct}}(t) = a e^{bt}$  ( $b > 0$ ) in continuous time, then the corresponding evolution in discrete time is given by  $x_{\text{dt}}(n) = a e^{c\tau n}$  with  $c = -(1/\tau) \log(1 - b\tau) > b$ . This implies that for systems that show unstable behaviour in continuous time, the instability is enhanced in the discrete-time context.

## CONCLUSIONS

To conclude, we have shown that the backward difference scheme preserves the non-negative character of the phase space density of a classical Hamiltonian system. The time evolution operator is a bounded operator for all times. We have shown that discretization of time leads to stochasticity. Irrespective of the number of degrees of freedom, one function of the phase space variables becomes stochastic. This variable has a unique probability density, which turns out to be the gamma density. The discrete-time evolution by a finite amount in the forward direction depends on the entire forward-time history of the continuous-time evolution. In this sense, the discrete-time evolution is nonlocal in time. The formula that relates  $\rho_{\text{dt}}(\vec{x}, \vec{p}, n)$  to  $\rho_{\text{ct}}(\vec{x}, \vec{p}, t)$  is suggestive of a random walk in an internal time. The motion of even free particles becomes correlated motion, in our formalism.

The same formalism is amenable to a quantum mechanical treatment via density matrices (equivalently, via the Wigner distribution functions). The elements of the density matrix that connect degenerate states are time-invariant, whereas the ones that connect non-degenerate states decay exponentially. Thus discretization of time leads to energy super-selection and decoherence in quantum mechanics. It is also interesting to note that an arrow of time emerges in the present framework. Finally, our approach does not seem to permit a consistent description of quantum mechanics via the discrete-time Schrödinger equation.

Some of the consequences of the discretization of time that we have pointed out in the foregoing are intriguing, and warrant further investigation to elucidate their meaning and implications. The complexities that may arise when the Liouville operator is not sufficiently ‘good’ should also be explored.

To conclude, classical stochasticity, quantum decoherence and an arrow of time emerge automatically in the present version of discrete-time mechanics. All these features disappear and we recover the usual classical and quantum mechanics in the limit  $\tau \rightarrow 0$ .

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### CALCULATION OF $g_n(\xi_1)$

We now proceed to calculate  $g_n(\xi_1)$  given by the relation

$$g_n(\xi_1) = \left( \frac{1 - \alpha\tau \partial/\partial\xi_1}{1 + \beta\tau \partial/\partial\xi_1} \right)^n \delta(\xi_1 - \xi_1(0)).$$

The Fourier transform  $\tilde{g}_n(k)$  of  $g_n(\xi_1)$  is given by

$$\tilde{g}_n(k) = \int_{-\infty}^{\infty} d\xi_1 e^{ik\xi_1} g_n(\xi_1) = \left( \frac{1 + i\alpha k}{1 - i\beta k} \right)^n e^{ik\xi_1(0)}.$$

Rewriting  $(1 + i\alpha k)/(1 - i\beta k)$  as  $\beta^{-1}[(1 - i\beta\tau k)^{-1} - \alpha]$  and using the binomial theorem, we get

$$\tilde{g}_n(k) = \left( \frac{1}{\beta} \right)^n \sum_{l=0}^n \binom{n}{l} (-\alpha)^{n-l} \left( \frac{1}{1 - i\beta\tau k} \right)^l e^{ik\xi_1(0)}. \quad (11)$$

Taking the inverse Fourier transform of Eq. (11), we get

$$g_n(\xi_1) = \left( -\frac{\alpha}{\beta} \right)^n \delta(\xi_1 - \xi_1(0)) + \left( \frac{1}{\beta} \right)^n \sum_{j=1}^n \binom{n}{j} (-\alpha)^{n-j} h_j(\xi_1), \quad (12)$$

where  $h_j(\xi_1)$  is given by the relation

$$h_j(\xi_1) = \begin{cases} \frac{(\beta\tau)^{-j}}{(j-1)!} (\xi_1 - \xi_1(0))^{j-1} \exp\left[-\frac{(\xi_1 - \xi_1(0))}{\beta\tau}\right], & \text{for } \xi_1 > \xi_1(0) \\ 0, & \text{for } \xi_1 < \xi_1(0). \end{cases}$$

In Eq. (12), the first term is singular, while the second is the sum of a finite number of regular functions. The first term is negative for odd  $n$ . It then follows that  $\alpha$  has to be zero for the probability density  $g_n(\xi_1)$  to be positive for all  $n$ . In that case  $g_n(\xi_1) = h_n(\xi_1)$ .

### TIME EVOLUTION OF $\rho_{dt}$

For forward evolution, i.e.,  $n > 0$ , define the generating function

$$G(\vec{x}, \vec{p}, z) = \sum_{n=0}^{\infty} z^n \rho_{dt}(\vec{x}, \vec{p}, n) = \sum_{n=0}^{\infty} z^n \left( \frac{1 + \alpha\tau L}{1 - \beta\tau L} \right)^n \rho_{dt}(\vec{x}, \vec{p}, 0),$$

to get

$$G(\vec{x}, \vec{p}, z) = \left( \frac{1 - \beta\tau L}{1 - z - (\beta + \alpha z)\tau L} \right) \rho_{dt}(\vec{x}, \vec{p}, 0).$$

This expression can be further simplified to

$$G(\vec{x}, \vec{p}, z) = \left( \frac{\beta}{\beta + \alpha z} \right) \rho_{dt}(\vec{x}, \vec{p}, 0) + \left( \frac{z}{\beta + \alpha z} \right) \left( \frac{1}{1 - z - (\beta + \alpha z)\tau L} \right) \rho_{dt}(\vec{x}, \vec{p}, 0).$$

Now use the integral representation

$$\begin{aligned} \frac{1}{1 - z - (\beta + \alpha z)\tau L} &= \int_0^{\infty} du \exp \{ -u [1 - z - (\beta + \alpha z)\tau L] \} \\ &= \sum_{m=0}^{\infty} \frac{z^m}{m!} (1 + \alpha\tau L)^m \int_0^{\infty} du u^m e^{-u} e^{\beta\tau L}, \end{aligned}$$

to get

$$G(x, p, z) = \left( \frac{\beta}{\beta + \alpha z} \right) \rho_{\text{dt}}(\vec{x}, \vec{p}, 0) + \left( \frac{z}{\beta + \alpha z} \right) \sum_{m=0}^{\infty} \frac{z^m}{m!} (1 + \alpha \tau L)^m \\ \times \int_0^{\infty} du u^m e^{-u} \rho_{\text{ct}}(\vec{x}, \vec{p}, \beta \tau u), \quad (13)$$

where  $\rho_{\text{ct}}(\vec{x}, \vec{p}, t)$  is the continuous-time phase space density given by Eq. (2). Collecting together the coefficients of  $z^n$  yields

$$\rho_{\text{dt}}(\vec{x}, \vec{p}, n) = \left( -\frac{\alpha}{\beta} \right)^n \rho_{\text{dt}}(\vec{x}, \vec{p}, 0) + \frac{1}{\beta} \sum_{j=0}^{n-1} \left( -\frac{\alpha}{\beta} \right)^{n-1-j} \frac{(1 + \alpha \tau L)^j}{j!} \\ \times \int_0^{\infty} du u^j e^{-u} \rho_{\text{ct}}(\vec{x}, \vec{p}, \beta \tau u). \quad (14)$$

The first term on the right-hand side in Eq. (14) is singular, and negative for odd  $n$ . The second is a sum of finite-order derivatives of a regular function. Therefore, in order for  $\rho_{\text{dt}}(\vec{x}, \vec{p}, n)$  to be non-negative,  $\alpha$  must vanish. Thus, both the methods referred to in the main text lead to the same answer. However, the second method yields the representation

$$\rho_{\text{dt}}(\vec{x}, \vec{p}, n) = \frac{1}{(n-1)!} \int_0^{\infty} du e^{-u} u^{n-1} \rho_{\text{ct}}(\vec{x}, \vec{p}, \tau u)$$

for  $\rho_{\text{dt}}(\vec{x}, \vec{p}, n)$  in terms of  $\rho_{\text{ct}}(\vec{x}, \vec{p}, t)$ .